



PTMProphetParser Usage:

USAGE: PTMProphetParser <OPTIONS> <input_file.pep.xml> [<output_file>]

OPTIONS

NOUPDATE Don't update modification_info tags in pepXML

EM=<number>: Set EM models to <number> which can be 0, 1, 2, or 3 (*default: 2*) :
0 -> no EM,
1 -> Intensity EM Model Applied Only,
2 -> Intensity and Matched Peaks EM Models Applied,
3 -> Matched Peaks EM Model Applied Only

KEEPOLD Option to retain old PTMProphet results in the pepXML file (*default: off*).

VERBOSE Option to produce WARNINGS to help troubleshoot potential PTM shuffling or mass difference issues (*default: off*).

STATIC Use static fragppmtol for all PSMs instead of dynamically estimates offsets and tolerances (*default: off*).

FRAGPPMTOL=<number> When computing PSM-specific mass_offset and mass_tolerance, use specified default +/- MS2 mz tolerance on fragment ions (*default: 15*).

PPMTOL=<number> Use specified +/- MS1 ppm tolerance on peptides which may have a slight offset depending on search parameters (e.g. iTRAQ4plex) (*default=1*).

MINPROB=<number> Use specified minimum probability to evaluate peptides (*default=0.9*).

MAXTHREADS=<number> Use specified number of threads for processing (*default=1*).

MASSDIFFMODE Treat the mass difference between measured and theoretical mass as a modification and localize

LABILITY Compute Lability of PTMs

DIRECT Use only direct evidence for evaluating PTM site probabilities

IFRAGS Use internal fragments for localization (*default: do not use internal fragments*)

AUTODIRECT Use direct evidence when the lability is high, use in combination with LABILITY

MAXFRAGZ=<integer> Limit maximum fragment charge (*default: precursor charge, negative values subtract from precursor charge*).

MINO=<integer> Use specified number of pseudo-counts when computing Oscore (*default=0*).

NOMINOFATOR Disable MINO factor correction when MINO= is set greater than 0 (*default: apply MINO factor correction*)

NIONS= Use specified N-term ions, separate multiple ions by commas (*default: a,b for CID, c for ETD*)

CIONS= Use specified C-term ions, separate multiple ions by commas (*default: y for CID, z for ETD*)

MASSOFFSET=<number> Adjust the massdiff by offset <number> (*default: 0*)

<amino acids, n, or c>:<mass_shift>:<neut_loss1>:....:<neut_lossN>,<amino acids, n, or c>:<mass_shift>:<neut_loss1>:....:<neut_lossN>

Specify modifications (*default: STY:79.9663,MW:15.9949*)

Supplemental Figure 2: This figure shows the complete USAGE statement of the PTMProphet software and default parameters, in yellow, utilized by PTMProphet.